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First principles prediction of a morphotropic phase boundary in the $Bi(Zn_{1/2}Ti_{1/2})O_3$-$(Bi_{1/2}Sr_{1/2})(Zn_{1/2}Nb_{1/2})O_3$ alloy[1] VALENTINO R. COOPER, Oak Ridge National Laboratory, ASEGUN S. HENRY, Georgia Institute of Technology, SHIGEYUKI TAKAGI, University of Tennessee, DAVID J. SINGH, Oak Ridge National Laboratory — We present a density functional theory study on alloys of the tetragonally distorted $Bi(Zn_{1/2}Ti_{1/2})O_3$ (BZT) and the rhombohedrally oriented $(Bi_{1/2}Sr_{1/2})(Zn_{1/2}Nb_{1/2})O_3$ (BSZN). We find that compositions with $\geq 50\%$ BZT are tetragonally distorted with the polarization pointing mainly along the [001] direction. Conversely, for low concentrations of BZT the polarization is rhombohedrally oriented. Based on these results we propose a phase diagram with a possible monoclinc phase between 25% and 50% BZT where this material may have a useful piezoelectric response.

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